Closures for coarse-grid simulation of fluidized gas-particle flows

Topic/Area of Interest: 11 – Coarse-grid modeling
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Project Summary

Context: Gas-particle flows in fluidized beds and riser reactors are inherently unstable, and they manifest fluctuations over a wide range of length and time scales. Two-fluid models for such flows reveal unstable modes whose length scale is as small as ten particle diameters. Yet, because of limited computational resources, gas-particle flows in large fluidized beds are invariably simulated by solving discretized versions of the two-fluid model equations over a coarse spatial grid. Such coarse-grid simulations do not resolve the small-scale spatial structures which are known to affect the macroscale flow structures both qualitatively and quantitatively. Thus there is a need to develop filtered two-fluid models which are suitable for coarse-grid simulations and capturing the effect of the small-scale structures through closures in terms of the filtered variables.

Proposed project: The overall objective of the project is to develop validated closures for filtered two-fluid models for gas-particle flows, with the transport gasifier as a primary, motivating example. In this project, highly resolved three-dimensional simulations of a kinetic theory based two-fluid model for gas-particle flows will be performed and the statistical information on structures in the 100-1000 particle diameters length scale will be extracted. Based on these results, closures for filtered two-fluid models will be constructed. The filtered model equations and closures will be validated against experimental data and the results obtained in highly resolved simulations of gas-particle flows.

Broad Impact: The proposed project will enable more accurate simulations of not only the transport gasifier, but also many other non-reacting and reacting gas-particle flows in a variety of chemical reactors. The results of this study will be in the form of closures which can readily be incorporated into existing multi-phase flow codes such as MFIX. Therefore, the benefits of this study can be realized quickly. The training provided by this project will prepare a PhD student to enter research and development careers in DOE laboratories or chemicals/energy-related industries.

Milestone for March 31, 2006: Demonstrate capability to gather region-averaged statistics from 3-D simulations of fluidization of uniformly sized particles in periodic domains.

Status on Milestone: We have indeed completed the code development required to extract statistics on various dynamic characteristics from highly resolved three-dimensional gas-particle flow simulations in periodic domains. We have completed a set of simulations and extracted the first set of results on how filtered drag coefficient, filtered particle phase pressure and viscosity vary with filter size and particle volume fraction for a typical gas-particle system. Our three-dimensional simulations in cubic domains led to results which are qualitatively similar to what we had seen previously in two-dimensional computations. We also found that quasi-three-dimensional simulations, where one of the horizontal directions was made smaller, yielded the same results as the simulations in cubic domains. This will therefore allow us to perform the future simulations in smaller domains with fewer numerical cells and hence faster computations.

Project Participant: Ms. Yesim Igci (graduate student at Princeton University) worked with the PI on this project. All the code development and analysis of results were performed by her.

Published Articles: We have not yet written any papers summarizing these results.

Completed/Future Presentations: The work mentioned above will be included in two presentations to be made by the PI in the next few weeks.

a) S. Sundaresan, A. T. Andrews IV & Yesim Igci, Coarse-graining two-fluid models for fluidized gas particle suspensions, The 231st ACS National Meeting, Atlanta, GA, March 28, 2006.
b) S. Sundaresan, A. T. Andrews IV, Yesim Igci, S. Pannala & T. O'Brien, Coarse-graining two-fluid models for fluidized gas particle suspensions, Fifth World Congress on Particle Technology, Orlando, FL, April 24, 2006.